Frank Abild-Pedersen

List of Publications by Year in Descending Order

167 papers	25,509 citations	66 h-index	159 g-index
182 ext. papers	29,593 ext. citations	9.7 avg, IF	7.12 L-index

#	Paper	IF	Citations
167	Colloidal Platinum-Copper Nanocrystal Alloy Catalysts Surpass Platinum in Low-Temperature Propene Combustion.. *Journal of the American Chemical Society*, **2022**,	16.4	2
166	Microkinetic Modeling of Propene Combustion on a Stepped, Metallic Palladium Surface and the Importance of Oxygen Coverage. *ACS Catalysis*, **2022**, 12, 1742-1757	13.1	2
165	Trends in oxygenate/hydrocarbon selectivity for electrochemical CO reduction to C products.. *Nature Communications*, **2022**, 13, 1399	17.4	6
164	Unraveling Electronic Trends in O* and OH* Surface Adsorption in the MO2 Transition-Metal Oxide Series. *Journal of Physical Chemistry C*, **2022**, 126, 7903-7909	3.8	0
163	Enhancing the connection between computation and experiments in electrocatalysis. *Nature Catalysis*, **2022**, 5, 374-381	36.5	4
162	Modeling Potential-Dependent Electrochemical Activation Barriers: Revisiting the Alkaline Hydrogen Evolution Reaction. *Journal of the American Chemical Society*, **2021**, 143, 19341-19355	16.4	7
161	Identification of earth-abundant materials for selective dehydrogenation of light alkanes to olefins. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	3
160	Theory-Aided Discovery of Metallic Catalysts for Selective Propane Dehydrogenation to Propylene. *ACS Catalysis*, **2021**, 11, 6290-6297	13.1	6
159	Ultrafast Adsorbate Excitation Probed with Subpicosecond-Resolution X-Ray Absorption Spectroscopy. *Physical Review Letters*, **2021**, 127, 016802	7.4	3
158	Dynamics and Hysteresis of Hydrogen Intercalation and Deintercalation in Palladium Electrodes: A Multimodal In Situ X-ray Diffraction, Coulometry, and Computational Study. *Chemistry of Materials*, **2021**, 33, 5872-5884	9.6	2
157	Achieving industrial ammonia synthesis rates at near-ambient conditions through modified scaling relations on a confined dual site. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	5
156	The role of atomic carbon in directing electrochemical CO(2) reduction to multicarbon products. *Energy and Environmental Science*, **2021**, 14, 473-482	35.4	25
155	Identifying factors controlling the selective ethane dehydrogenation on Pt-based catalysts from DFT based micro-kinetic modeling. *Journal of Energy Chemistry*, **2021**, 58, 37-40	12	1
154	Combining artificial intelligence and physics-based modeling to directly assess atomic site stabilities: from sub-nanometer clusters to extended surfaces. *Physical Chemistry Chemical Physics*, **2021**, 23, 22022-22034	3.6	3
153	The Role of Roughening to Enhance Selectivity to C2+ Products during CO2 Electroreduction on Copper. *ACS Energy Letters*, **2021**, 6, 3252-3260	20.1	4
152	Bimetallic effects on Zn-Cu electrocatalysts enhance activity and selectivity for the conversion of CO2 to CO. *Chem Catalysis*, **2021**, 1, 663-680		11
151	Guiding the Catalytic Properties of Copper for Electrochemical CO Reduction by Metal Atom Decoration. *ACS Applied Materials & Interfaces*, **2021**,	9.5	2

150	Efficient Screening of Bimetallic Electrocatalysts for Glycerol Valorization. *Electrochimica Acta*, **2021**, 398, 139283	6.7	1
149	Insights and comparison of structure–property relationships in propane and propene catalytic combustion on Pd- and Pt-based catalysts. *Journal of Catalysis*, **2021**, 401, 89-101	7.3	4
148	Revealing the structure of a catalytic combustion active-site ensemble combining uniform nanocrystal catalysts and theory insights. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 14721-14729	11.5	10
147	Predicting metal-metal interactions. II. Accelerating generalized schemes through physical insights. *Journal of Chemical Physics*, **2020**, 152, 094702	3.9	5
146	Accuracy of XAS theory for unraveling structural changes of adsorbates: CO on Ni(100). *AIP Advances*, **2020**, 10, 115014	1.5	3
145	Enhanced CO tolerance of Pt clusters supported on graphene with lattice vacancies. *Physical Review B*, **2020**, 102,	3.3	8
144	From electricity to fuels: Descriptors for C1 selectivity in electrochemical CO2 reduction. *Applied Catalysis B: Environmental*, **2020**, 279, 119384	21.8	37
143	Predicting metal-metal interactions. I. The influence of strain on nanoparticle and metal adlayer stabilities. *Journal of Chemical Physics*, **2020**, 152, 094701	3.9	5
142	Machine Learning for Computational Heterogeneous Catalysis. *ChemCatChem*, **2019**, 11, 3581-3601	5.2	127
141	Revealing the Synergy between Oxide and Alloy Phases on the Performance of Bimetallic In–Pd Catalysts for CO2 Hydrogenation to Methanol. *ACS Catalysis*, **2019**, 9, 3399-3412	13.1	105
140	Predicting Adsorption Properties of Catalytic Descriptors on Bimetallic Nanoalloys with Site-Specific Precision. *Journal of Physical Chemistry Letters*, **2019**, 10, 1852-1859	6.4	28
139	Enhancing Electrocatalytic Water Splitting by Strain Engineering. *Advanced Materials*, **2019**, 31, e1807001	14	240
138	Supported Catalyst Deactivation by Decomposition into Single Atoms Is Suppressed by Increasing Metal Loading. *Nature Catalysis*, **2019**, 2,	36.5	99
137	Understanding Structure-Property Relationships of MoO-Promoted Rh Catalysts for Syngas Conversion to Alcohols. *Journal of the American Chemical Society*, **2019**, 141, 19655-19668	16.4	16
136	A coordination-based model for transition metal alloy nanoparticles. *Nanoscale*, **2019**, 11, 4438-4452	7.7	23
135	Accessing the C-C transition state energy on transition metals. *Physical Chemistry Chemical Physics*, **2019**, 21, 25328-25333	3.6	1
134	Structure-Sensitive Scaling Relations: Adsorption Energies from Surface Site Stability. *ChemCatChem*, **2018**, 10, 1643-1650	5.2	38
133	Generic approach to access barriers in dehydrogenation reactions. *Communications Chemistry*, **2018**, 1,	6.3	6

132	Selectivity of Synthesis Gas Conversion to C2+ Oxygenates on fcc(111) Transition-Metal Surfaces. *ACS Catalysis*, **2018**, 8, 3447-3453	13.1	48
131	Theoretical Investigation of Methane Oxidation on Pd(111) and Other Metallic Surfaces. *Journal of Physical Chemistry C*, **2018**, 122, 16023-16032	3.8	21
130	Spin Uncoupling in Chemisorbed OCCO and CO2: Two High-Energy Intermediates in Catalytic CO2 Reduction. *Journal of Physical Chemistry C*, **2018**, 122, 12251-12258	3.8	12
129	Low-Temperature Methane Partial Oxidation to Syngas with Modular Nanocrystal Catalysts. *ACS Applied Nano Materials*, **2018**, 1, 5258-5267	5.6	13
128	A Highly Active Molybdenum Phosphide Catalyst for Methanol Synthesis from CO and CO2. *Angewandte Chemie*, **2018**, 130, 15265-15270	3.6	12
127	A Highly Active Molybdenum Phosphide Catalyst for Methanol Synthesis from CO and CO. *Angewandte Chemie - International Edition*, **2018**, 57, 15045-15050	16.4	46
126	Nature of Lone-Pair-Surface Bonds and Their Scaling Relations. *Inorganic Chemistry*, **2018**, 57, 7222-7238	5.1	35
125	Comparison of Sintering by Particle Migration and Ripening through First-Principles-Based Simulations. *Journal of Physical Chemistry C*, **2018**, 122, 26563-26569	3.8	8
124	Theoretical and Experimental Studies of CoGa Catalysts for the Hydrogenation of CO2 to Methanol. *Catalysis Letters*, **2018**, 148, 3583-3591	2.8	9
123	Strongly Modified Scaling of CO Hydrogenation in Metal Supported TiO Nanostripes. *ACS Catalysis*, **2018**, 8, 10555-10563	13.1	6
122	Tuning Methane Activation Chemistry on Alkaline Earth Metal Oxides by Doping. *Journal of Physical Chemistry C*, **2018**, 122, 22544-22548	3.8	13
121	Mechanistic Insights into the Synthesis of Higher Alcohols from Syngas on CuCo Alloys. *ACS Catalysis*, **2018**, 8, 10148-10155	13.1	39
120	Mechanistic insights into heterogeneous methane activation. *Physical Chemistry Chemical Physics*, **2017**, 19, 3575-3581	3.6	72
119	Scaling Relations for Adsorption Energies on Doped Molybdenum Phosphide Surfaces. *ACS Catalysis*, **2017**, 7, 2528-2534	13.1	30
118	Modeling the Migration of Platinum Nanoparticles on Surfaces Using a Kinetic Monte Carlo Approach. *Journal of Physical Chemistry C*, **2017**, 121, 4261-4269	3.8	25
117	Catalysis in real time using X-ray lasers. *Chemical Physics Letters*, **2017**, 675, 145-173	2.5	35
116	Electrochemical generation of sulfur vacancies in the basal plane of MoS for hydrogen evolution. *Nature Communications*, **2017**, 8, 15113	17.4	396
115	A Theoretical Study of Methanol Oxidation on RuO2(110): Bridging the Pressure Gap. *ACS Catalysis*, **2017**, 7, 4527-4534	13.1	5

114	Bond Order Conservation Strategies in Catalysis Applied to the NH3 Decomposition Reaction. *ACS Catalysis*, **2017**, 7, 864-871	13.1	19
113	Configurational Energies of Nanoparticles Based on Metal–Metal Coordination. *Journal of Physical Chemistry C*, **2017**, 121, 23002-23010	3.8	27
112	Systematic Structure–Property Relationship Studies in Palladium-Catalyzed Methane Complete Combustion. *ACS Catalysis*, **2017**, 7, 7810-7821	13.1	110
111	Investigating Catalyst–Support Interactions To Improve the Hydrogen Evolution Reaction Activity of Thiomolybdate [Mo3S13]2– Nanoclusters. *ACS Catalysis*, **2017**, 7, 7126-7130	13.1	55
110	Theoretical Insights into Methane C–H Bond Activation on Alkaline Metal Oxides. *Journal of Physical Chemistry C*, **2017**, 121, 16440-16446	3.8	34
109	Real-Time Elucidation of Catalytic Pathways in CO Hydrogenation on Ru. *Journal of Physical Chemistry Letters*, **2017**, 8, 3820-3825	6.4	7
108	Rh-MnO Interface Sites Formed by Atomic Layer Deposition Promote Syngas Conversion to Higher Oxygenates. *ACS Catalysis*, **2017**, 7, 5746-5757	13.1	49
107	Understanding trends in C-H bond activation in heterogeneous catalysis. *Nature Materials*, **2017**, 16, 225–229	27	276
106	Two-Dimensional Materials as Catalysts for Energy Conversion. *Catalysis Letters*, **2016**, 146, 1917-1921	2.8	39
105	Chemical Bond Activation Observed with an X-ray Laser. *Journal of Physical Chemistry Letters*, **2016**, 7, 3647-51	6.4	15
104	Direct and continuous strain control of catalysts with tunable battery electrode materials. *Science*, **2016**, 354, 1031-1036	33.3	369
103	Methanol Partial Oxidation on Ag(1 1 1) from First Principles. *ChemCatChem*, **2016**, 8, 3621-3625	5.2	10
102	Dynamical Observation and Detailed Description of Catalysts under Strong Metal-Support Interaction. *Nano Letters*, **2016**, 16, 4528-34	11.5	160
101	Elucidating the electronic structure of supported gold nanoparticles and its relevance to catalysis by means of hard X-ray photoelectron spectroscopy. *Surface Science*, **2016**, 650, 24-33	1.8	14
100	Chemical and Phase Evolution of Amorphous Molybdenum Sulfide Catalysts for Electrochemical Hydrogen Production. *ACS Nano*, **2016**, 10, 624-32	16.7	86
99	Activating and optimizing MoS2 basal planes for hydrogen evolution through the formation of strained sulphur vacancies. *Nature Materials*, **2016**, 15, 48-53	27	1563
98	Computational catalyst screening: Scaling, bond-order and catalysis. *Catalysis Today*, **2016**, 272, 6-13	5.3	35
97	Modeling the Interface of Platinum and α-Quartz(001): Implications for Sintering. *Journal of Physical Chemistry C*, **2016**, 120, 10340-10350	3.8	17

96	Trends in the Thermodynamic Stability of Ultrathin Supported Oxide Films. *Journal of Physical Chemistry C*, **2016**, 120, 10351-10360	3.8	19
95	Sintering of Pt Nanoparticles via Volatile PtO2: Simulation and Comparison with Experiments. *ACS Catalysis*, **2016**, 6, 7098-7108	13.1	52
94	The Mechanism of CO and CO2 Hydrogenation to Methanol over Cu-Based Catalysts. *ChemCatChem* , **2015**, 7, 1105-1111	5.2	336
93	Engineering high-performance Pd core-MgO porous shell nanocatalysts via heterogeneous gas-phase synthesis. *Nanoscale*, **2015**, 7, 13387-92	7.7	16
92	Examining the Linearity of Transition State Scaling Relations. *Journal of Physical Chemistry C*, **2015**, 119, 10448-10453	3.8	18
91	Strong Influence of Coadsorbate Interaction on CO Desorption Dynamics on Ru(0001) Probed by Ultrafast X-Ray Spectroscopy and Ab□nitio Simulations. *Physical Review Letters*, **2015**, 114, 156101	7.4	22
90	Predicting Promoter-Induced Bond Activation on Solid Catalysts Using Elementary Bond Orders. *Journal of Physical Chemistry Letters*, **2015**, 6, 3670-4	6.4	12
89	Surface Tension Effects on the Reactivity of Metal Nanoparticles. *Journal of Physical Chemistry Letters*, **2015**, 6, 3797-801	6.4	52
88	Designing an improved transition metal phosphide catalyst for hydrogen evolution using experimental and theoretical trends. *Energy and Environmental Science*, **2015**, 8, 3022-3029	35.4	671
87	Rational design of MoS2 catalysts: tuning the structure and activity via transition metal doping. *Catalysis Science and Technology*, **2015**, 5, 246-253	5.5	128
86	Hydrogenation of CO2 to methanol and CO on Cu/ZnO/Al2O3: Is there a common intermediate or not?. *Journal of Catalysis*, **2015**, 328, 43-48	7.3	186
85	From the Sabatier principle to a predictive theory of transition-metal heterogeneous catalysis. *Journal of Catalysis*, **2015**, 328, 36-42	7.3	715
84	Toward Controlled Growth of Helicity-Specific Carbon Nanotubes. *Journal of Physical Chemistry Letters*, **2015**, 6, 2232-7	6.4	6
83	On the role of the surface oxygen species during A-H (A = C, N, O) bond activation: a density functional theory study. *Chemical Communications*, **2015**, 51, 2621-4	5.8	38
82	Surface chemistry. Probing the transition state region in catalytic CO oxidation on Ru. *Science*, **2015** , 347, 978-82	33.3	150
81	Theoretical insights into the hydrogen evolution activity of layered transition metal dichalcogenides. *Surface Science*, **2015**, 640, 133-140	1.8	256
80	Transition-metal doped edge sites in vertically aligned MoS2 catalysts for enhanced hydrogen evolution. *Nano Research*, **2015**, 8, 566-575	10	478
79	Insights into carbon nanotube nucleation: cap formation governed by catalyst interfacial step flow. *Scientific Reports*, **2014**, 4, 6510	4.9	35

78	Tuning the MoS edge-site activity for hydrogen evolution via support interactions. *Nano Letters*, **2014**, 14, 1381-7	11.5	533
77	Discovery of a Ni-Ga catalyst for carbon dioxide reduction to methanol. *Nature Chemistry*, **2014**, 6, 320-4	17.6	689
76	Effects of d-band shape on the surface reactivity of transition-metal alloys. *Physical Review B*, **2014**, 89,	3.3	236
75	Activity and Selectivity Trends in Synthesis Gas Conversion to Higher Alcohols. *Topics in Catalysis*, **2014**, 57, 135-142	2.3	144
74	Understanding the Reactivity of Layered Transition-Metal Sulfides: A Single Electronic Descriptor for Structure and Adsorption. *Journal of Physical Chemistry Letters*, **2014**, 5, 3884-9	6.4	57
73	Inherent Enhancement of Electronic Emission from Hexaboride Heterostructure. *Physical Review Applied*, **2014**, 2,	4.3	16
72	Catalysis. Assessing the reliability of calculated catalytic ammonia synthesis rates. *Science*, **2014**, 345, 197-200	33.3	244
71	Theoretical Analysis of Transition-Metal Catalysts for Formic Acid Decomposition. *ACS Catalysis*, **2014**, 4, 1226-1233	13.1	169
70	Active edge sites in MoSe2 and WSe2 catalysts for the hydrogen evolution reaction: a density functional study. *Physical Chemistry Chemical Physics*, **2014**, 16, 13156-64	3.6	364
69	Electronic Structure Effects in Transition Metal Surface Chemistry. *Topics in Catalysis*, **2014**, 57, 25-32	2.3	154
68	DFT Study of Atomically-Modified Alkali-Earth Metal Oxide Films on Tungsten. *Journal of Physical Chemistry C*, **2014**, 118, 11303-11309	3.8	12
67	**2014**,		219
66	Catalyst Structure **2014**, 138-149		
65	Poisoning and Promotion of Catalysts **2014**, 150-154		
64	Energy Trends in Catalysis **2014**, 85-96		1
63	The Electronic Factor in Heterogeneous Catalysis **2014**, 114-137		8
62	Activity and Selectivity Maps **2014**, 97-113		0
61	Operando Characterization of an Amorphous Molybdenum Sulfide Nanoparticle Catalyst during the Hydrogen Evolution Reaction. *Journal of Physical Chemistry C*, **2014**, 118, 29252-29259	3.8	66

60	The Potential Energy Diagram **2014**, 6-25		
59	Energetics of the Water–Gas-Shift Reaction on the Active Sites of the Industrially Used Cu/ZnO/Al2O3 Catalyst. *Catalysis Letters*, **2014**, 144, 1973-1977	2.8	23
58	Exploring the limits: A low-pressure, low-temperature Haber–Bosch process. *Chemical Physics Letters*, **2014**, 598, 108-112	2.5	275
57	Interlayer carbon bond formation induced by hydrogen adsorption in few-layer supported graphene. *Physical Review Letters*, **2013**, 111, 085503	7.4	87
56	Analysis of sulfur-induced selectivity changes for anhydrous methanol dehydrogenation on Ni(100) surfaces. *Surface Science*, **2013**, 613, 58-62	1.8	4
55	Stability of Pt-Modified Cu(111) in the Presence of Oxygen and Its Implication on the Overall Electronic Structure. *Journal of Physical Chemistry C*, **2013**, 117, 16371-16380	3.8	4
54	On the effect of coverage-dependent adsorbate–adsorbate interactions for CO methanation on transition metal surfaces. *Journal of Catalysis*, **2013**, 307, 275-282	7.3	160
53	Electronic Origin of the Surface Reactivity of Transition-Metal-Doped TiO2(110). *Journal of Physical Chemistry C*, **2013**, 117, 460-465	3.8	72
52	CO and CO2 Hydrogenation to Methanol Calculated Using the BEEF-vdW Functional. *Catalysis Letters*, **2013**, 143, 71-73	2.8	122
51	Comment on "Using Photoelectron Spectroscopy and Quantum Mechanics to Determine d-Band Energies of Metals for Catalytic Applications". *Journal of Physical Chemistry C*, **2013**, 117, 6914-6915	3.8	13
50	Brønsted–Evans–Polanyi Relationship for Transition Metal Carbide and Transition Metal Oxide Surfaces. *Journal of Physical Chemistry C*, **2013**, 117, 4168-4171	3.8	56
49	Investigation of Catalytic Finite-Size-Effects of Platinum Metal Clusters. *Journal of Physical Chemistry Letters*, **2013**, 4, 222-6	6.4	221
48	Thermionic current densities from first principles. *Journal of Chemical Physics*, **2013**, 138, 204701	3.9	8
47	In silicosearch for novel methane steam reforming catalysts. *New Journal of Physics*, **2013**, 15, 125021	2.9	55
46	Elementary steps of syngas reactions on Mo2C(001): Adsorption thermochemistry and bond dissociation. *Journal of Catalysis*, **2012**, 290, 108-117	7.3	84
45	Application of a new informatics tool in heterogeneous catalysis: Analysis of methanol dehydrogenation on transition metal catalysts for the production of anhydrous formaldehyde. *Journal of Catalysis*, **2012**, 291, 133-137	7.3	39
44	CatApp: A Web Application for Surface Chemistry and Heterogeneous Catalysis. *Angewandte Chemie*, **2012**, 124, 278-280	3.6	26
43	CatApp: a web application for surface chemistry and heterogeneous catalysis. *Angewandte Chemie - International Edition*, **2012**, 51, 272-4	16.4	106

42	Energetics of Oxygen Adatoms, Hydroxyl Species and Water Dissociation on Pt(111). *Journal of Physical Chemistry C*, **2012**, 116, 25772-25776	3.8	54
41	CO hydrogenation to methanol on Cu□Ni catalysts: Theory and experiment. *Journal of Catalysis*, **2012**, 293, 51-60	7.3	163
40	A theoretical evaluation of possible transition metal electro-catalysts for N2 reduction. *Physical Chemistry Chemical Physics*, **2012**, 14, 1235-45	3.6	810
39	Reversible graphene-metal contact through hydrogenation. *Physical Review B*, **2012**, 86,	3.3	25
38	The active site of methanol synthesis over Cu/ZnO/Al2O3 industrial catalysts. *Science*, **2012**, 336, 893-7	33.3	1650
37	Metal Oxide-Supported Platinum Overlayers as Proton-Exchange Membrane Fuel Cell Cathodes. *ChemCatChem*, **2012**, 4, 228-235	5.2	42
36	Volcano Relations for Oxidation of Hydrogen Halides over Rutile Oxide Surfaces. *ChemCatChem*, **2012**, 4, 1856-1861	5.2	11
35	An orbital-overlap model for minimal work functions of cesiated metal surfaces. *Journal of Physics Condensed Matter*, **2012**, 24, 445007	1.8	22
34	Universal transition state scaling relations for (de)hydrogenation over transition metals. *Physical Chemistry Chemical Physics*, **2011**, 13, 20760-5	3.6	295
33	Scaling relationships for adsorption energies of C2 hydrocarbons on transition metal surfaces. *Chemical Engineering Science*, **2011**, 66, 6318-6323	4.4	93
32	Density functional theory in surface chemistry and catalysis. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 937-43	11.5	1141
31	Universal Br□sted-Evans-Polanyi Relations for C□, C□, C□, N□, N□, and O□ Dissociation Reactions. *Catalysis Letters*, **2011**, 141, 370-373	2.8	215
30	Descriptor-Based Analysis Applied to HCN Synthesis from NH3 and CH4. *Angewandte Chemie*, **2011**, 123, 4697-4701	3.6	11
29	Descriptor-based analysis applied to HCN synthesis from NH3 and CH4. *Angewandte Chemie - International Edition*, **2011**, 50, 4601-5	16.4	68
28	On the behavior of Br□sted-Evans-Polanyi relations for transition metal oxides. *Journal of Chemical Physics*, **2011**, 134, 244509	3.9	108
27	First-principles investigations of Ni3Al(111) and NiAl(110) surfaces at metal dusting conditions. *Surface Science*, **2011**, 605, 582-592	1.8	10
26	Structure effects on the energetics of the electrochemical reduction of CO2 by copper surfaces. *Surface Science*, **2011**, 605, 1354-1359	1.8	368
25	Electrochemical chlorine evolution at rutile oxide (110) surfaces. *Physical Chemistry Chemical Physics*, **2010**, 12, 283-90	3.6	244

24	On the Role of Metal Step-Edges in Graphene Growth. *Journal of Physical Chemistry C*, **2010**, 114, 11221-11227	4.8	102
23	Volcano Relation for the Deacon Process over Transition-Metal Oxides. *ChemCatChem*, **2010**, 2, 98-102	5.2	48
22	How copper catalyzes the electroreduction of carbon dioxide into hydrocarbon fuels. *Energy and Environmental Science*, **2010**, 3, 1311	35.4	1861
21	Self Blocking of CO Dissociation on a Stepped Ruthenium Surface. *Topics in Catalysis*, **2010**, 53, 357-364	2.3	42
20	Trends for Methane Oxidation at Solid Oxide Fuel Cell Conditions. *Journal of the Electrochemical Society*, **2009**, 156, B1447	3.9	15
19	First-principles investigations of the Ni3Sn alloy at steam reforming conditions. *Surface Science*, **2009**, 603, 762-770	1.8	37
18	Structure sensitivity of the methanation reaction: H2-induced CO dissociation on nickel surfaces. *Journal of Catalysis*, **2008**, 255, 6-19	7.3	365
17	First principles calculations and experimental insight into methane steam reforming over transition metal catalysts. *Journal of Catalysis*, **2008**, 259, 147-160	7.3	488
16	The nature of the active site in heterogeneous metal catalysis. *Chemical Society Reviews*, **2008**, 37, 2163-71	38.5	553
15	Identification of non-precious metal alloy catalysts for selective hydrogenation of acetylene. *Science*, **2008**, 320, 1320-2	33.3	795
14	Using scaling relations to understand trends in the catalytic activity of transition metals. *Journal of Physics Condensed Matter*, **2008**, 20, 064239	1.8	80
13	Scaling relationships for adsorption energies on transition metal oxide, sulfide, and nitride surfaces. *Angewandte Chemie - International Edition*, **2008**, 47, 4683-6	16.4	260
12	On the role of surface modifications of palladium catalysts in the selective hydrogenation of acetylene. *Angewandte Chemie - International Edition*, **2008**, 47, 9299-302	16.4	197
11	Scaling Relationships for Adsorption Energies on Transition Metal Oxide, Sulfide, and Nitride Surfaces. *Angewandte Chemie*, **2008**, 120, 4761-4764	3.6	49
10	On the Role of Surface Modifications of Palladium Catalysts in the Selective Hydrogenation of Acetylene. *Angewandte Chemie*, **2008**, 120, 9439-9442	3.6	33
9	Carbide induced reconstruction of monatomic steps on Ni(1 1 1) – A density functional study. *Surface Science*, **2007**, 601, 649-655	1.8	11
8	CO adsorption energies on metals with correction for high coordination adsorption sites – A density functional study. *Surface Science*, **2007**, 601, 1747-1753	1.8	207
7	Scaling properties of adsorption energies for hydrogen-containing molecules on transition-metal surfaces. *Physical Review Letters*, **2007**, 99, 016105	7.4	1009

6	Mechanisms for catalytic carbon nanofiber growth studied by ab initio density functional theory calculations. *Physical Review B*, **2006**, 73,	3.3	229
5	Methane activation on Ni(1 1 1): Effects of poisons and step defects. *Surface Science*, **2005**, 590, 127-137	1.8	211
4	Understanding the Effect of Steps, Strain, Poisons, and Alloying: Methane Activation on Ni Surfaces. *Catalysis Letters*, **2005**, 105, 9-13	2.8	67
3	Atomic-scale imaging of carbon nanofibre growth. *Nature*, **2004**, 427, 426-9	50.4	1195
2	DFT Study of Formaldehyde and Methanol Synthesis from CO and H2 on Ni(111)□ *Journal of Physical Chemistry B*, **2004**, 108, 14535-14540	3.4	98
1	Exploring Trends on Coupling Mechanisms toward C3 Product Formation in CO(2)R. *Journal of Physical Chemistry C*,	3.8	4